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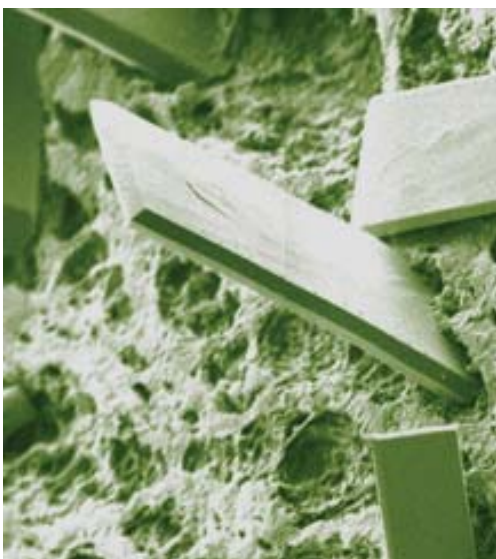
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# Design and analysis of membrane based process intensification and hybrid processing options

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## Introduction

The paper covers model-based design and analysis as well as experiment-based verification and analysis within the context of process intensification and hybrid processing. Process intensification (PI) as well as hybrid processing has the potential to improve existing processes or create new process options, which are needed in order to produce products using more sustainable methods. Recently, process intensification (PI) has been defined as the improvement of a whole process through enhancements of the involved phenomena in terms of the following PI-principles: (a) integration of unit operations, (b) integration of functions, (c) integration of phenomena, (d) targeted enhancements of phenomena in a given operation. Hybrid processing, could therefore, also be considered as a special option within PI (a).

Membrane based approaches can provide an essential contribution to this technology. For example, operations such as electromembrane filtration, in which the transport phenomena are enhanced by adding electrophoretic transport phenomena, as an alternative method for the fractionation of enzymes. Another example is the integration of membrane based operations with biocatalytic (enzyme based conversions) or biotransformation (resting cell based conversions) or fermentation (growing cell based conversions). Since bioprocesses are often limited to an unfavorable equilibrium or inhibition, this integration can be used to overcome the limitations by *in-situ* product removal (ISPR) or *in-situ* substrate supply (ISSS).

Even though promising, identification and/or development of membrane based PI and hybrid process options are not simple. Therefore, a model-based design method is beneficial to quickly and systematically identify, to analyze and to select promising candidates, which can then be investigated in detail, including experimental verification. In this way, the integration of modeling and experiments is time and resources saving since the experimental effort can be exploited for verification rather than for identification of potential candidates. Additionally, models can be used to appropriately design the type of experiments to be performed.

The objective of this paper is to present methodologies for model-based design and analysis as well as experiment-based verification within the context of PI and hybrid processing.

## Theory

### a) Phenomena-based PI synthesis/design methodology

A phenomena-based PI synthesis/design approach has been developed for quick identification, generation and evaluation of PI process options. It is based on two contributions [1]: a) the use of phenomena building blocks (models) together with connection equations to represent a process; b) the use of a decomposition solution approach for efficient solving of the complex mathematical optimization problem. Starting from the problem definition (step 1), suitable phenomena to match the defined target are identified based on analysis of the process (step 2). In step 3, the methodology generates a set of process options and reduces their number to the feasible and structural promising options. In step 4, the search space is further reduced by hierarchical screening by operational constraints and a performance metrics. In step 5, the remaining options are optimized with respect to the defined objective for identification of the optimal process option. The main advantage of this approach is that it can generate potentially novel process options (truly predictive models are

required to generate reliable solutions) as well as the simultaneous development of the necessary process models. The application of the methodology together with necessary tools/algorithms developed for it is highlighted through case study 1.

#### **b) Hybrid process design methodology**

This developed knowledge-based methodology is aimed to identify the best possible hybrid process configuration for reaction-separation (R-S) and separation-separation (S-S) systems given desired targets for process improvement. The methodology consists of three stages [2]: (1) hybrid process design and analysis, (2) process implementation (including experimental setup) and (3) process-model validation.

The design and analysis objective is to systematically identify the potential separation and reaction techniques as well as the process conditions that fulfill the desired design improvements. For that purpose, the system is analyzed at the separation and reaction levels. A list of feasible combinations leads to feasible hybrid process schemes for S-S and R-S. From there, the hybrid process schemes can be evaluated as well as the quality of the models verified.

A key contribution within this framework is the generic mass and energy models employed to create the flowsheet superstructure plus the separation process models library. The membrane based processes incorporated in the library are: gas separation, pervaporation, vacuum membrane distillation, sweeping gas membrane distillation, direct contact membrane distillation, osmotic membrane distillation, solvent nanofiltration and reverse osmosis.

#### **c) Methodology for design of a novel integrated membrane bioreactor**

In order to evaluate the potential of a novel membrane bioreactor technology under development, a model-based approach supported by experimental evidence has shown to be useful to understand the controlled operation of the integrated process. This is required due to the challenges at both the design and control levels for integrated systems. A simple systematic procedure has been developed as a first attempt to study integrated process operation. It allows the preliminary evaluation of potential production improvements and identification of integration issues [3].

The complexity of the models, model validity constraints and potential infeasible simulation scenarios of the integrated system, increase the complexity of a simultaneous control and process design. Therefore, the solution of the integration problem is attempted in a sequential manner while accounting for the conceptual interaction between design and control of the integrated process.

The design strategy is aimed to exploit the unit interaction for both productivity enhancement and process control purposes. Through dynamic model analysis, the unit roles can be identified according to certain production goal. This permits incorporating regulatory control layers to the process design. This decomposition strategy makes possible to design the integrated process and investigate the system operation only on the interest regions of the operating window, avoiding undesired simulation scenarios and attempting solving the model at unfeasible process conditions. The application of this methodology is illustrated in case study 2.

### **Results**

#### **Case study 1: Continuous production of isopropyl-acetate**

The phenomena-based PI synthesis/design methodology is highlighted through the continuous production of isopropyl-acetate from isopropanol and acetic-acid.

In step 1, the objective is to identify the process at lowest operational costs and capital costs for the production of 50.000t/a of isopropyl-acetate. Additional performance criteria are the yield, energy and volume. In step 2, information of the process is collected and analyzed based on pure-component, mixture and reaction properties. The reaction analysis identifies the limitation of the reaction by and unfavorable equilibrium. The following phenomena were identified for the process:

mixing (ideal), dividing phenomena, heating/ cooling (countercurrent, co-current, conductive), heterogeneous reaction and phase split. Additionally, the promising phase separations of products from reactants are identified to be based on Vapor-Liquid separation (boiling points) or pervaporation (radius of gyration).

In step 3, all these phenomena are combined using connectivity rules and the information of the operational window. The identified phenomena were connected to form phenomena-based flowsheets (72315 options) using connectivity rules and subsequently screened by additional logical and structural constraints to identify the set of feasible and structural promising options (194). Examples of four of these options are highlighted in Fig. 1.

In step 4, all phenomena-based options are screened by operational constraints and afterwards transformed to unit operation using rules since some operational constraints and performance constraints are related to the physical unit (such as the volume). In total 23, options are remaining in the search space. Examples of identified units from generated phenomena-based flowsheets and involved phenomena are shown in Fig. 1. The performance of the generated flowsheets is evaluated using the product yield (A: 0.65, B: 0.99, C: 0.80 and D: 0.99), where options B and D are found to be equally good. In step 5, the best option is identified through solving a reduced optimization problem which is plate-membrane/heat-exchanger reactor.

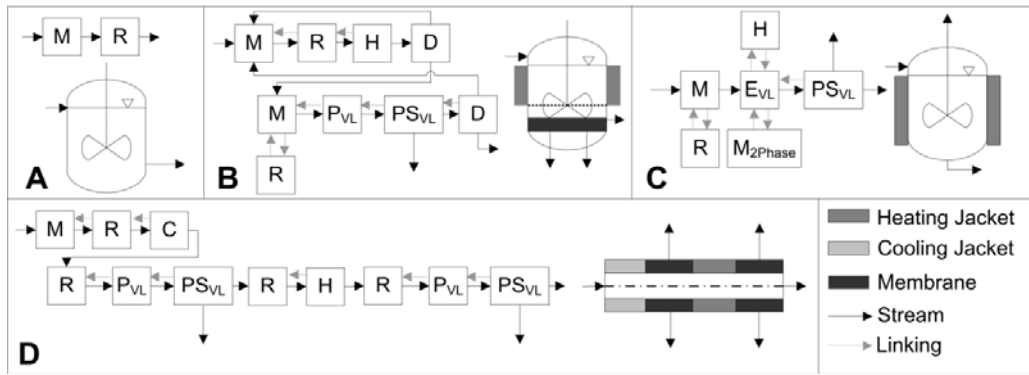


Figure 1. Identified flowsheets: (A) single phase CSTR; (B) CSTR with integrated heating jacket and membrane; (C) Isothermal Reactive Flash; integrated membrane, thermal controlled tubular reactor. Phenomena: Ideal mixing M; Reaction R; Phase creation: pervaporation P, evaporation E; phase separation PS, Heating H, Cooling C and Dividing D. Utility streams for energy supply/removal are not shown.

### Case study 2: Membrane bioreactor design for lactic acid fermentation

A simple methodology to investigate coupled process and control design of an integrated bioreactor with a novel electrically driven membrane separation process (Reverse Electro-Enhanced Dialysis - REED) is proposed. The methodology uses previously developed rigorous models for the unit operations [3]. The REED module continuously exchanges the biotoxic lactate, from the fermentation broth, by hydroxyl ions. Therefore, it reduces the adverse influence of the product inhibition and facilitates the pH control in the fermenter.

The first step is the definition of the process goal, the case study is the batch production of a starter culture. Secondly, the roles of the tightly coupled units are defined. The integrated system is designed in the scenario where the REED module role is to regulate the pH at maximum bioreactor productivity. For this purpose, a decentralized pH control structure is implemented using PI controllers in an input-resetting control structure. The complete pH control structure of the integrated system is depicted in Fig. 2. At this stage, the bioreactor is designed according to the separation capabilities of the REED unit. This strategy allows integrating the models. Finally, in



order to reveal the potential benefit of process integration it is relevant to compare the performance of conventional batch fermentation (simulated), with batch fermentation coupled with electrodialysis (experimental, [4]) and with the integrated fermentation and REED system (simulated). The investigation reveals that a design of REED can partially facilitate the pH control in the fermenter. The final biomass concentration, biomass yield and productivity are substantially increased in the REED process compared to the batch fermentation and an integrated fermentation and electrodialysis (120% biomass productivity enhancement compared to electrodialysis case).

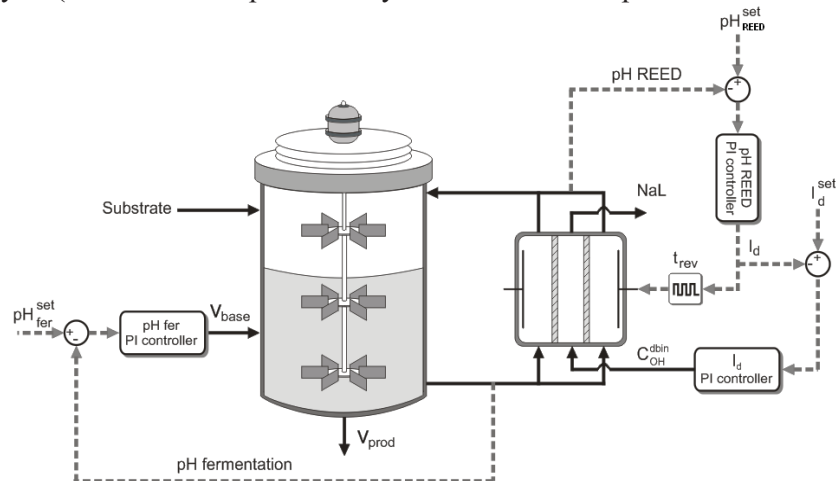


Figure 2. Sketch of the complete pH control architecture of the integrated system. Solid lines are flow streams while dashed lines are signals. The input resetting control structure controls the separation in REED while there is a PI pH controller in the fermenter

## Conclusions

The paper highlights the collection of generic models developed within the design methodologies. Besides, model-based systematic methodologies for design and analysis of PI and hybrid processing options are presented. Finally, application of the models and the design method is highlighted through case studies, where potential intensified processes are identified and interaction between unit operations is exploited during the design stage.

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